Adv. Studies Theor. Phys., Vol. 7, 2013, no. 14, 685 - 686
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http://dx.doi.org/10.12988/astp.2013.3547

A Simple Way for Obtaining the Expression for the Entropy of Fluid

II. The Random Phase Approximation

Anatoliy Yuryev[1,2]

[1)] Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia
[2)] Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences,
Amundsen st. 101, 620016 Ekaterinburg, Russia
yurev_anatolii@mail.ru

Nikolay Dubinin[1,2]

[1)] Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia
[2)] Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences,
Amundsen st. 101, 620016 Ekaterinburg, Russia
ned67@mail.ru

Vladimir Filippov[1,2]

[1)] Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia
[2)] Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences,
Amundsen st. 101, 620016 Ekaterinburg, Russia
vvfilippov@mail.ru

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Abstract

The more simple technique is used to obtain the analytical expression of the entropy for the square-well fluid in the random phase approximation.

Keywords: Entropy, square-well fluid, random phase approximation

In the previous article (I) was shown a more simple way to obtain the entropy, *S*, of an equilibrium arbitrary fluid with the hard-core (HC) pair potential,

$$\varphi_{\mathrm{HC}}(r)=\begin{cases}\infty, & r<\sigma\\ \phi(r), & r\geq\sigma\end{cases}\quad . \tag{1}$$

Here, we apply this way to the square-well (SW) model within the random phase approximation (RPA) [1]. The attractive part of $\varphi_{\mathrm{SW}}(r)$ is

$$\phi_{\mathrm{SW}}(r)=\begin{cases}0, & r<\sigma\\ \varepsilon, & \sigma\leq r<\lambda\sigma\\ 0, & r\geq\lambda\sigma\end{cases}\quad , \tag{2}$$

where ε, λ and σ are the SW parameters.

Then, Fourier transform of Eq. (2) is

$$\phi_{\mathrm{SW}}(q)=\frac{4\pi\varepsilon}{q^{3}}\left[\sin(q\lambda\sigma)-\sin(q\sigma)-q\lambda\sigma\cos(q\lambda\sigma)+q\sigma\cos(q\sigma)\right]\quad . \tag{3}$$

The expression for the Fourier transform of the direct correlation function, $c(r)$, in the SW-RPA approach is

$$c_{\mathrm{SW\text{-}RPA}}(q)=c_{\mathrm{HS}}(q)-\beta\phi_{\mathrm{SW}}(q)\,, \tag{4}$$

where $\beta=(k_{\mathrm{B}}T)^{-1}$, T is the absolute temperature, k_{B} - Boltzmann constant, $c_{\mathrm{HS}}(q)$ - the Fourier transform of the direct correlation function in the hard-sphere (HS) model for which there is the analytical expression [2]. The structure factor, $a(q)$, of the SW system within the RPA is written as

$$a_{\mathrm{SW\text{-}RPA}}(q)=\frac{1}{1-\rho c_{\mathrm{HS}}(q)+\beta\rho\phi_{\mathrm{SW}}(q)}\quad . \tag{5}$$

Finally, using Eq.(10) from (I) we have the following expression for the entropy:

$$S_{\mathrm{SW\text{-}RPA}}=S_{\mathrm{HS}}+\frac{k_{\mathrm{B}}}{4\pi^{2}}\int_{0}^{\infty}dq\,q^{2}\left(\beta a_{\mathrm{SW\text{-}RPA}}(q)\phi_{\mathrm{SW}}(q)+\frac{1}{\rho}\ln\frac{a_{\mathrm{SW\text{-}RPA}}(q)}{a_{\mathrm{HS}}(q)}\right), \tag{6}$$

where $a_{\mathrm{HS}}(q)=1/\left(1-\rho c_{\mathrm{HS}}(q)\right)$, ρ - mean atomic density.

Since the expression for $a_{\mathrm{SW\text{-}RPA}}(q)$ is known, Eq.(6) can be used for actual calculations.

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Received: April 30, 2013